NERL/AMD Publications

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Jan 1, 2000 - Dec 31, 2000

Presented Published

ABSTRCT/ORAL

Binkowski, F.S., Roselle, S.J., Eder, B.K., and Mebust, M.R. Evaluation of predicted visual range using the community multiscale air quality modeling system. Presented at: European Aerosol Conference, Dublin, Ireland, September 3-8, 2000. 9/3/2000

Contact: Francis S. Binkowski

Abstract:

Schere, K.L., Roselle, S.J., and Binkowski, F.S. U.S. EPA's multi-pollutant Models-3/community multi-scale air quality model. Presented at: NARSTO Tropospheric Aerosols Symposium, Queretaro, Mexico, October 25, 2000. 10/25/2000

Contact: Shawn J. Roselle

Abstract:

Byun, D.W. EPA's Models-3: community multiscale air quality (CMAQ) modeling system. Presented at: Air Quality Symposium, Houston, TX, September 29, 2000. 9/29/2000

Contact: Daewon W. Byun

Abstract:

Bullock, O.R. The importance of emissions speciation to the atmospheric transport and deposition of mercury. Presented at: EPA Conference on Assessing and Managing mercury from Historic and Current Mining Activities, San Francisco, CA, November 28-30, 2000. 11/28/2000

Contact: Russell Bullock

Abstract: The atmospheric pathway of the global mercury cycle is believed to be the main source of mercury contamination to aquatic eco-systems throughout the United States and in most other nations where direct disposal of mercury to water has been largely eliminated. Although the spatial scope of transport and deposition is certainly global for atmospheric mercury as a whole, we now have compelling evidence that certain forms of mercury are very quickly scavenged from air by both wet and dry atmospheric processes and are not likely to travel very long distances through the atmosphere. Reactive gaseous mercury (RGM) and particulate mercury (HgP), while together making up only a small fraction of the total atmospheric burden of mercury, are thought to represent the majority of atmospheric mercury deposited to the surface. Mercury can be emitted to air in one of these forms, and travel only a short distance before deposition, or it can be emitted as elemental mercury gas (Hg0) and move through the atmosphere for weeks or months, diffusing into the global atmosphere. Based on recent modeling and field studies, it now appears that most of the elemental mercury that is eventually deposited to the surface may do so through chemical conversion to RGM and/or particulate mercury. It also appears that emissions of RGM and HgP can be converted to Hg0 by these same atmospheric processes under different conditions. While there remains considerable uncertainty about these chemical and physical conversion mechanisms, the expected deposition pattern for mercury from any source is certainly dependent on the chemical and physical form of that mercury when emitted. The term "speciation" is generally used to describe the determination of the fraction of a pollutant that occurs in various important forms. Mercury emission speciation is necessary for an assessment of mercury contamination from any source of atmospheric mercury.

Huber, A.H., Singh, R.B., Gilliam, R.C., and Braddock, J.N. Real-time modeling and measurement of mobile source pollutant concentrations for estimating human exposures in communities near roadways. Presented at: 2000 Annual Meeting of the International Society of Exposure Analysis, Pacific Grove, CA, October 24-27, 2000. 10/24/2000

Contact: William B. Petersen

Abstract: The United States Environmental Protection Agency's (EPA) National Exposure Research Laboratory (NERL) is pursuing a project to improve the methodology for real-time site specific modeling of human exposure to pollutants from motor vehicles. The overall project goal is to develop improved methods for modeling the source through the air pathway to human exposure in significant microenvironments of exposure. Our developments for microscale modeling refer to spatial scales from the size of an individual vehicle to the order of 1 km. Current human exposure models using simplified assumptions based on a few fixed air monitoring stations or modeled concentrations from regional-scale motor vehicle emission/transport models have great uncertainty in representing the actual human exposures and should be improved. The first component of the modeling framework is real-time site-specific motor vehicle emission models capable of capturing real-world emissions. Then an urban-scale meteorological and air dispersion model is used to provide ambient air concentrations resulting from transport and other human activities. Refined modeling using Computational Fluid Dynamics (CFD) simulation is being applied to develop refined air dispersion models for linkage to a roadway microenvironmental model. This modeling framework helps in establishing the direct relationships between source-to-exposure specific to the particular exposure microenvironment (e.g., standing by the roadside or actually inside the vehicle, inside the moving vehicle, living nearby a roadway). The complete modeling framework from source-to-exposure together with some measurements carried out in the Research Triangle Park area of North Carolina is shown to be a viable system that can be transferred to other locations both as real-time support for an ongoing human exposure field study or to develop feasible scenarios to build distributions of key parameters for a human exposure model.

Singh, R.B., Huber, A.H., and Braddock, J.N. Real-time modeling of motor vehicle emissions for estimating human exposures near roadways. Abstract presented at: 2000 Annual Meeting of the International Society of Exposure Analysis, Pacific Grove, CA, October 24-27, 2000. 10/24/2000

Contact: William B. Petersen

Abstract:

Huber, A.H., Bolstad, M., Rida, S., Bish, I.E.S., and Kuehlert, K.H. Addressing human exposures to air pollutants around buildings in urban areas with computational fluid dynamics models. Presented at: AMS Third Symposium on the Urban Environment, Davis, CA, August 14-18, 2000. 8/14/2000

Contact: William B. Petersen

Abstract: This paper discusses the status and application of Computational Fluid Dynamics (CFD) models to address challenges for modeling human exposures to air pollutants around urban building microenvironments. There are challenges for more detailed understanding of air pollutant source emissions, transport and dispersion, and the resulting human exposures. The application of CFD for detailed modeling of urban building microenvironments requires tools for complex geometry creation and meshing, advanced physical models, parallel computing capabilities and scientific visualization. CFD simulations are able to account rigorously for details of buildings and structures in urban areas as well as local aerodynamics and turbulence. These features can be influential in determining local human exposures to environmental pollution. CFD simulation of complex distributions of pollutant concentration within microenvironments of human exposure are feasible using today's high performance computing. Output from CFD can be directly used to both simulate real events and provide a better understanding of exposure events than is now available from any other modeling method. In some cases the output of CFD simulations can be used in the tunnel study measurements have been used. Wind tunnel studies can be used to provide validation data for the CFD simulations for the limited physical conditions that may be studied in a wind tunnel. CFD modeling allows for the inclusion of complex physical processes such as turbulence, chemical reactions, heat and mass transfer. Through further research, validation and testing, CFD modeling has the potential to become a reliable tool for estimating pollutant concentrations for situations that today have no reliable modeling method. Discussions with examples are presented to highlight the use of CFD simulations as a tool for addressing human exposures around buildings in urban areas. Particular attention is given to geometry modeling and meshing, the application of physical models and parameters (e.g., boundary conditions and turbulence models) and simulation post processing and evaluation.

Jan 1, 2000 - Dec 31, 2000

Presented Published

Lawson, Jr., R.E., Thompson, R.S., Perry, S.G., and Snyder, W.H. Modeling puff diffusion in a laboratory. 11th Joint Conference on the Applications of Air Pollution Meteorology with the AWMA, Long Beach, CA, January 9-14, 2000. 1/19/2000

Contact: Steven G. Perry

Abstract:

Kuehlert, K.H., Bish, I.E.S., and Huber, A.H. Addressing environmental engineering challenges with computational fluid dynamics. Presented at: AWMA 93rd Annual Meeting and Exhibition, Salt Lake City, UT, June 18-22, 2000. 6/18/2000

Contact: William B. Petersen

Abstract: In the field of environmental engineering, modeling tools are playing an ever larger role in addressing air quality issues, including source pollutant emissions, atmospheric dispersion and human exposure risks. More detailed modeling of environmental flows requires tools for complex geometry creation and meshing, advanced physical models and parallel computing capabilities. Computational fluid dynamics (CFD) simulations provide a number of unique opportunities for expanding and improving capabilities for modeling environmental flows.

Singh, R.B., Huber, A.H., and Braddock, J.N. Development of a microscale emission factor model for particulate matter (MicroFacPM) for predicting real time motor vehicle emissions. Presented at: PM 2000 AWMA Conference, Charleston, SC, January 24-28, 2000. 1/25/2000

Contact: William B. Petersen

Abstract: Health risk evaluation needs precise measurement and modeling of human exposures in microenvironments to support review of current air quality standards. The particulate matter emissions from motor vehicles are a major component of human exposures in urban microenvironments. Current human exposure models using simplified assumptions based on fixed air monitoring stations and regional scale emission models do not represent the actual human exposures and should be improved. A number of independent studies have found that present mobi8le sources particulate emission factor models are not reliable at estimating microscale human exposures in-vehicles and near roadways. The particulate emission factor model PART5 (used in USA except California) and EMFAC (used in California only) calculate the composite emission factors for each vehicle class by weighting the emission factors calculated for each model year by the travel fraction for that model year and then summing the weighted factors. This method is suitable for regional scale emission estimates and for emission invntory, but not for emission factor estimates in microenvironments needed for human exposure models. In view of the above, a micro-scale emission factor model (MicroFacPM) for predicting real-time automobile PM 10 and PM 2.5 emissions is being developed, using the same database that was used to develop part 5. The algorithm used to calculate emission factorsIn MicroFacPM is disaggregated. It calculates emission factors in real-time form the on-road vehicle fleet. MicroFacPM fully accounts for exhaust and non-exhaust (such as tire wear, break wear and re-entrained road dust) sources and can also be used near roadway intersections. The model can be applied to estimate emission factors for fleet of vehicles between January 1, 1990, and December 31, 2010, and therefore allows a comparison of current emissions with past and future, or in a contribution of particulate matter from different sources. Microfacpm will be an important tool to characterize the relationship between fixed site monitors and actual human exposures in different microenvironments near roadways. The model is also appropriate for comparative analyses; for example, comparing the potential impact of one traffic control measure versus another.

Presented *Published*

Singh, R.B., and Huber, A.H. Development of a model for real time CO concentrations near roadways. Presented at: AWMA 93rd Annual Meeting and Exhibition, Salt Lake City, UT, June 18-22, 2000. — 6/18/2000

Contact: William B. Petersen

Abstract: Although emission standards for mobile sources continue to be tightened, tailpipe emissions in urban areas continue to be a major source of human exposure to air toxics. Current human exposure models using simplified assumptions based on fixed air monitoring stations and regional scale emission models do not represent the actual human exposures and should be improved. The MOBILE (used in USA except California) and EMFAC(used in California only) mobile source emission models are suitable for supporting regional scale modeling and emission inventory. These emission models have not be designed to estimated real-time emissions needed to support human exposure studies near roadways. A number of independent studies have found that these emission factor models are not reliable for estimating microscale emissions and therefore inappropriate to be used with roadway dispersion models and microenvironmental modeling necessary to estimate human exposures near roadways. Therefore, it has become necessary to design a real-time emission factor model capable of estimating emission factors at microscale level helpful in establishing complex source-to dose relationships. In view of the above, a real time microscale automobile emission factor model for CO (MicroFacCo), virtually capturing all the information in the real world, has been developed for United States vehicles. The algorithm used to calculate emission factors is disaggregated based on the on-road vehicle fleet. The emission factors are calculated from a real-time fleet, not for a fleet-wide average estimated by vehicle miles traveled (VMT) weighting of the emission factors for different vehicle classes (methodology used to develop MOBILE and EMFAC). MicroFacCo calculates the emission factors from a road on a lane-by-lane basis and for available vehicle fleet structure data based on direct observations, video records, available tunnel studies vehicle fleet or average values of the country or region. Apart from calculating composite emission factors, the model also gives the contribution of CO from different sources, both depending on vehicle class wise and year wise. The model is being used to conjunction with roadway dispersion models (i.e.CALINE4), and being evaluated in the roadways around research triangle park, north carolina in a range of traffic fleet and meteorological conditions. Modeled concentrations are bing compared with measured concentrations inside a vehicle and along the roadside of I-40 and highway 70.

Schwede, D.B., and Petersen, W.B. Simulating atmospheric exposure using an innovative meteorological sampling scheme. Presented at: NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 15-19, 2000. — 5/15/2000

Contact: William B. Petersen

Abstract: Multimedia risk assessments require the temporal integration of atmospheric concentration and deposition with other media modules. However, providing an extended time series of estimates is computationally expensive. An alternative approach is to substitute long-term average atmospheric estimates, but traditional methods for calculating long-term averages are not amendable to estimating wet deposition. In an effort to produce the required estimates without the computational burden, we developed an extension to the Sampled Chronological Imputed Model (SCIM) for use in ISCST3. SCIM samples the long term meteorological record at regular, user-specified intervals. Since hourly meteorology is being used, the serial correlation between wet deposition and concentration is maintained. Our results show that, for a 5 year meteorological-database, sampling every 193rd hour produced concentration and dry deposition estimates essentially the same as those obtained when using the full meteorological record. However, this simple sampling scheme significantly underestimated wet deposition, particularly at sites with infrequent precipitation. For wet deposition, the key to the success of SCIM is the addition of an additional sampling interval (every 8th hour)for hours with precipitation . this approach resulted in wet deposition estimates that were not significantly different than those obtained from the full record. The development of this innovative sampling approach has resulted in an efficient methodology for use in multimedia risk assessments.

Weil, J.C., Snyder, W.H., Lawson, Jr., R.E., and Shipman, M.S. New development in dispersion experiments and models for the convective boundary layer. Presented at: NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 15-19, 2000. 5/15/2000

Contact: William B. Petersen

Abstract: We present recent experiments and modeling studies of dispersion in the convective boundary layer (CBL) with focus on highly-buoyant plumes that "loft" near the CBL top and resist downward mixing. Such plumes have been a significant problem in earlier dispersion models; they are defined by dimensionless buoyancy fluxes F 0.1, where F =Fb/(Uw ?z), Fb is the source buoyancy flux, U is the mean wind speed, w is the convective velocity scale, and the z is the CBL depth. The chief experimental aim is to obtain statistically reliable mean and fluctuating concentration fields as a function of F and a dimensionless distance X. The experiments are conducted in a convection tank similar to that used by Willis and Deardorff (1987), but with markedly improved data acquisition techniques and statistics.

Cooter, E.J., and Cohen, Y. A dynamic simulator of environmental chemical partitioning. Presented at: 2000 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, CA, November 12-17, 2000. 11/12/2000

Contact: William B. Petersen

Abstract: A version of the Community Multiscale Air Quality (CMAQ) model has been developed by the U.S. EPA that is capable of addressing the atmospheric fate, transport and deposition of some common trace toxics. An initial, 36-km rectangular grid-cell application for atrazine has been developed for the United States and southern Canada for a continuous 120 day period during the Spring and Summer of 1995. The principle focus of the analysis is Lake Michigan and its surrounding watershed. Grid-cell average model results are compared to total ambient atmospheric measurements reported by the U.S. EPA Lake Michigan Mass Balance (LMMB) Study and the USGS National Weather Quality Assessment program for 1995. Grid-averaged weekly and monthly aggregate wet deposition model results are compared to observations reported by the LMMB, USGS and Environment Canada. Special attention is given to gas/particle partitioning mechanisms when modeling ambient atmospheric concentration since expected partitioning behavior, based only on direct particle sorption, does not appear to adequately explain most field observations. Inclusion of additional sorption mechanisms (i.e., liquid film and film pH) results in model estimates that more closely resemble reported values. In the future, a second, 12 km rectangular grid domain, centered over Lake Michigan itself, will be nested within the larger model domain for a sub-set of the 120 day period to obtain more spatially resolved wet and dry chemical deposition patterns over the Lake surface.

Cooter, E.J., and Hutzell, W.T. Regional modeling of the atmospheric transport and deposition of atrazine. Presented at: Society of Environmental Toxicology and Chemistry 21st Annual Meeting, Nashville, TN, November 12-16, 2000. 11/12/2000

Contact: William B. Petersen

Abstract: A version of the Community Multiscale Air Quality (CMAQ) model has been developed by the U.S. EPA that is capable of addressing the atmospheric fate, transport and deposition of some common trace toxics. An initial, 36-km rectangular grid-cell application for atrazine has been developed for the United States and southern Canada for a continuous 120 day period during the Spring and Summer of 1995. The principle focus of the analysis is Lake Michigan and its surrounding watershed. Grid-cell average model results are compared to total ambient atmospheric measurements reported by the U.S. EPA Lake Michigan Mass Balance (LMMB) Study and the USGS National Weather Quality Assessment program for 1995. Grid-averaged weekly and monthly aggregate wet deposition model results are compared to observations reported by the LMMB, USGS and Environment Canada. Special attention is given to gas/particle partitioning mechanisms when modeling ambient atmospheric concentration since expected partitioning behavior, based only on direct particle sorption, does not appear to adequately explain most field observations. Inclusion of additional sorption mechanisms (i.e., liquid film and film pH) results in model estimates that more closely resemble reported values. In the future, a second, 12 km rectangular grid domain, centered over Lake Michigan itself, will be nested within the larger model domain for a sub-set of the 120 day period to obtain more spatially resolved wet and dry chemical deposition patterns over the Lake surface.

Jan 1, 2000 - Dec 31, 2000

Presented Published

Hutzell, W.T. Factors influencing the deposition of a compound that partitions between gas and particulate phases. Presented at: Fall 2000 Meeting of the American Geophysical Union, San Francisco, CA, December 15-19, 2000. 12/15/2000

Contact: William T. Hutzell

Abstract: How will atmospheric deposition behave for a compound when it reversibly sorbs between gas and atmospheric particulate phases? Two factors influence the answer. What physical mechanisms occur in the sorption process? What are the concentration and composition of atmospheric particulate matter that is the sorbent? The factors combine to produce deposition behaviors associated with both phases. They also infer a dependence on the compound's physical properties and meteorological variables such as temperature and humidity. The result makes difficult identifying what phase dominates atmospheric deposition at any time or location. Numerical modeling is a method that can qualitatively define the changes in deposition versus this dominance. This research investigates how sorption affects deposition by using an Eulerian model for particulate matter and deposition. The model includes an algorithm that partitions mass between gas and particulate phases based on equilibrium isotherms for sorption. The algorithm, itself, depends on concentrations of simulated particulate matter and includes parameters that control a compound's potential to sorb onto particulate matter. In the investigation, these parameters are varied to examine the effects on wet and dry deposition, separately. The results provide insights on how deposition changes when the ratio changes between concentrations in gas and particulate phases. The information may support future modeling of compounds that undergo the gas to particulate sorption. Several such compounds are relevant in assessing environmental health.

Hutzell, W.T. Model development and testing for semi-volatiles (Atrazine). Presented at: 1999 POP and Heavy Metals Workshop, Durham, NC, October 10-11, 1999. 10/10/2000

Contact: William T. Hutzell

Abstract: The Community Multi-Scale Air Quality (CMAQ) model, air quality model within EPA's Models-3 system, can be adapted to simulate the fate of semi-volatile compounds that are emitted into the atmosphere. "Semi-volatile" refers to compounds that partition their mass between two phases within the atmosphere. One phrase is gaseous. The other phase is sorbed onto atmospheric particulate matter. The fate of such compounds has relevance toward assessing environmental health because several toxic compounds fall into the category. This presentation discusses progress in adapting CMAQ to simulate atmospheric concentrations and deposition of semi-volatile compounds. It first outlines changes to the model to accomplish the goal. The presentation then focuses on applying the revised model to Atrazine, a widely used agricultural pesticide. The application illustrates how concentrations in gas and sorbed phases change based on the algorithm used to partition mass between the phases. The result implies that water vapor greatly affects the partitioning Atrazine. The presentation concludes on future research and model development that will improve modeling Atrazine and other semi-volatile compounds.

Poole-Kober, E.M. Atmospheric Sciences Modeling Division library poster. Presented at: SAIL 2000: Harness the Power of Information, 10th Annual Meeting, U.S. EPA, Research Triangle Park, NC, April 5-7, 2000. 4/5/2000

Contact: Evelyn Poole-kober

Abstract:

Poole-Kober, E.M. SAIL (Southeast Affiliate of IAMSLIC) poster. Presented at: SAIL 2000: Harness the Power of Information, 10th Annual Meeting, U.S. EPA, Research Triangle Park, NC, April 5-7, 2000. 4/5/2000

Contact: Evelyn Poole-kober

Abstract:

Landis, M.S., Stevens, R.K., Luke, W., and Keeler, G.J. Investigating the influence of long range transport on mercury deposition in south Florida. Abstract presented at: International Conference on Heavy Metals in the Environment, Ann Arbor, MI, August 6-10, 2000. 8/6/2000

Contact: Bruce W. Gay

Abstract:

Pierce, Jr., T.E., Kinnee, E.J., and Geron, C.D. Development of a 1-km vegetation database for modeling biogenic fluxes of hydrocarbons and nitric oxide. Presented at: Sixth International Conference on Air Surface Exchange of Gases and Particles, Edinburgh, England, July 3-7, 7/3/2000

Contact: Thomas E. Pierce

Abstract:

Gilliland, A.B., Pierce, Jr., T.E., Dennis, R.L., and Roselle, S.J. Inverse modeling to estimate seasonal ammonia emissions. Presented at: Shared Resources Workshop-Airsheds and Watersheds: The Significance of Ammonia to Coastal and Estuarine Areas, Dewey Beach, DE, November 15-16, 2000. 11/15/2000

Contact: Alice Gilliland

Abstract:

LeDuc, S.K., Schere, K.L., Godowitch, J.M., and Gipson, G.L. Models-3/CMAQ applications which illustrate capability and functionality. Presented at: Millennium NATO/CMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 15-19, 2000. 5/15/2000

Contact: Sharon K. Leduc

Abstract: The Models-3/CMAQ developed by the U.S. Environmental Protections Agency (USEPA) is a third generation multiscale, multi-pollutant air quality modeling system within a high-level, object-oriented computer framework (Models-3). It has been available to the scientific community since July 1998 with annual releases since that date. The system was designed to be flexible and modular. The science has been documented (USEPA, 1999a) and a user guide prepared for the framework (USEPA, 1999b). Current users of Models-3/CMAQ have tried various options in their applications, some of which will be shared at the First Annual Models-3 Workshop to be held in June 2000 (http://www.epa.gov/asmdnerl/models3). The Models-3/CMAQ has considerable capability at this time. The user may select from multiple chemical mechanisms which are provided as well as edit or revise those mechanisms. Two chemical mechanisms have been evaluated thus far in Models-3/CMAQ: RADM2 and Carbon Bond IV. Emissions for these mechanisms are generated using the Models-3 Emission Processing and Projection System (MEPPS). MEPPS can be executed using the framework "Study Planner" (USEPA, 1999b) which directs and monitors multiple execution steps. MEPPS which invokes both SAS and ARC/INFO can also be executed outside the framework. Emission control strategies can be developed within the MEPPS or can be created outside MEPPS by adjusting emission files. The latter approach was used to simulate uniform emission reductions as described on the poster. A Plume-in-Grid capability is also available in Models-3/CMAQ which contains a Lagrangian reactive plume model to simulate subgrid scale pollutant plumes from major point sources within an Eulerian grid. Plume concentrations are integrated into the concentration in a grid cell after the plume segment reaches model grid size.

Open-source visualization tools, Vis5D (http://www.ssec.wisc.edu/ billh/vis5d.html), PAVE(http://envpro.ncsc.org/OTAGDC/pave_letter.html) and Data Explorer (DX), (http://www.research.ibm.com/dci/software.html) are integrated into the Models-3/CMAQ and are used for analyzing and displaying the results. Evaluations of the accuracy and patterns of the simulations have been done using SAS. The Model-3 framework requires either a Sun workstation, Windows NT on a PC, or Silicon Graphics workstation. The framework Study Planner allows for model simulations to be conducted on computer platforms other than the one running the framework. The science codes will execute on other computing platforms and model execution can be performed on various platforms by using scripts without the Models-3 framework. However, the user must manually make changes in the script that would otherwise be made by the framework. Cray computers, both vector and parallel, have been successfully used with the standalone scripts as well as with the Study Planner in the system framework.

Presented Published

Solomon, P.A., Chameides, W.L., Edgerton, E.S., Scheffe, R.D., and Vanderpool, R.W. Objectives, design, and preliminary results from the Atlanta supersite project. Presented at: Real World 2000, Clean Air Conference, Atlanta, GA, May 15-18, 2000. 5/1/2000

Contact: Basil Dimitriades

Abstract: Objectives, Design, and Preliminary Results from The Atlanta Supersite ProjectPaul A. Solomon*, US EPA, ORD/NERL, MD-46, RTP, NC 27711 (solomon.paul@epa.gov) William Chameides, Georgia Institute of Technology, Atlanta, GA 30332 Eric Edgerton, ARA, Inc., Durham, NC 27702 Rich Scheffe, US EPA, OAQPS, RTP, NC, 27711 Robert Vanderpool, RTI, RTP, NC 27709 *Corresponding author.The Atlanta Supersites project is the first of two Supersites projects to be established during Phase I of EPA's Supersites Program; Phase II is being established through a Request for Assistance. The other initial project is in Fresno, California. The Supersite Program is part of EPA's National PM2.5 network, which consists of about 1100 sites for PM2.5 mass measured by the FRM and about 250-300 sites where the major components of PM2.5 will be determined. The objectives of the Supersites Program are to obtain information on atmospheric processes and provide information to assist states with State Implementation Plans (SIPS) for PM2.5, to support health effects related studies, and to evaluate measurement methods for particulate matter (PM) and PM precursors. The Atlanta Supersites project is focused on the last of these objectives, but meets the other objectives through leveraging with ongoing studies, including the Southeastern Aerosol Research Characterization Study (SEARCH), Aerosol Research Inhalation Epidemiological Study (ARIES), Southern Center For the Integrated Study of Secondary Air Pollutants (SCISSAP), and others. Specifically, evaluations at Atlanta focused on state-of-the-science measurement methods for PM and PM precursors and related species. Methods evaluated as part of the Atlanta Supersite project included four single particle mass spectrometer type methods, a series of semicontinuous methods for mass, sulfate, nitrate, ammonium, gas phase counter parts and other related species, and integrated filter/denuder based methods for PM2.5 mass and the chemical components of mass. Sampling occurred over a 28 day period during the month of August at a SEARCH/AREIS site located in NE Atlanta. This paper will describe the objectives and design of the Atlanta Supersite project and present preliminary results, where available.This work has been funded wholly or in part by the United States Environmental Protection Agency through internal funding. It has been subjected to Agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.Submitted for presentation at the Real World 2000 Clean Air Conference.

JOURNAL

Schere, K.L., and Hidy, G. Foreword NARSTO critical reviews - Atmospheric Environment. March 2000. Atmospheric Environment 34 (12-14):1853-1860 (2000). EPA/600/J-01/265. 2/7/2000

Contact: Kenneth L. Schere

Abstract: The last scientific assessment of our state of knowledge of the physical and chemical sciences relevant to the tropospheric ozone pollution issue in the United States was performed in 1991 by the U.S. National Research Council (NRC), and resulted in the report, Rethinking the Ozone Problem in Urban and Regional Air Pollution. In the ensuing years since its publication, a considerable investment has been made by both public and private interests in new field, laboratory and modeling programs focused on the further understanding of tropospheric ozone. In addition, based in part on a recommendation contained in the NRC report, the North American Research Strategy for Tropospheric Ozone (NARSTO) was formed with over 70 participating organizations from three nations involved in tropospheric ozone research. This current effort represents the first assessment under the NARSTO auspices, and the first attempt at doing so from a "complete" North American perspective. The work represents a major update of the 1991 NRC report, and focuses on progress of ozone science in the light of changing priorities in the regulatory environment not only in the U.S. but also in Canada and Mexico. As a part of the NARSTO Assessment, 24 critical reviews of various disciplinary science components were prepared that are relevant to the basic understanding, analysis and management of tropospheric ozone. The reviews are grouped topically and are interrelated. Authors of the reviews are experts in their fields who served as synthesizers of the new information generated by many investigators over the past decade. They were selected by the standing NARSTO Analysis and Assessment Team, in conjunction with the sponsors of the particular review. This series of reviews provided information for the 1999 NARSTO Assessment Report (An Assessment of Tropospheric Ozone Pollution: A North American Perspective, NARSTO, 1999). This report explores the extent to which current scientific understanding addresses the major contemporary issues of tropospheric ozone in air quality management.

Zhang, Y., Seigneur, C., Seinfeld, J.H., Jacobson, M.Z., Clegg, S.L., and Binkowski, F.S. A comparative review of inorganic aerosol thermodynamic equilibrium modules: similarities, differences, and their likely causes. November 1999. Atmospheric Environment 34 (1):117-137 (2000). EPA/600/J-00/031. 1/1/2000

Contact: Francis S. Binkowski

Abstract: A comprehensive comparison of five inorganic aerosol thermodynamic equilibrium modules, MARS-A, SEQUILIB, SCAPE2, EQUISOLV II, and AIM2, was conducted for a variety of atmospheric concentrations of particulate matter (PM) constituents, relative humidities (RHs), and temperatures. Our results show that although the PM compositions and concentrations predicted by these modules are generally comparable under most conditions, significant discrepancies exist under some conditions, especially at high nitrate/chloride concentrations and low/medium Rhs. As a consequence, the absolute differences in total PM concentrations predicted by these modules under all simulation conditions are 7.7-12.3% on average and as much as 68% for specific cases. The PM predictions are highly sensitive to changes in the molar ratios of ammonium to sulfate, nitrate to sulfate, and sodium chloride to sulfate, relative humidity, and temperature. The similarities and differences in simulation results predicted by the five modules are analyzed and the likely causes for these differences are discusses in detail. Recommendations are provided regarding the relative advantages of these modules, possible improvements of their performance, and applications in three-dimensional PM modeling studies.

Bullock, O.R. Current methods and research strategies for modeling atmospheric mercury. 2000. Fuel Processing Technology 65-66 (0):459-471 (2000). EPA/600/J-00/261. 7/1/2000

Contact: Russell Bullock

Abstract: The atmospheric pathway of the global mercury cycle is known to be the primary source of mercury contamination to most threatened aquatic ecosystems. Current efforts toward numerical modeling of atmospheric mercury are hindered by an incomplete understanding of emissions, atmospheric transformations, and deposition processes. While much effort has been made to quantify the total mass flux of mercury to the atmosphere from various natural and anthropogenic sources, discrimination of the chemical and physical forms of these emissions is just beginning in response to early modeling exercises showing this discrimination to be critical for accurate modeling estimates of the sources responsible for observed mercury deposition. A similar discrimination of ambient concentrations of mercury throughout the atmosphere is needed in order to develop a clear understanding of atmospheric transformation processes, both chemical and physical, which govern the length scale of atmospheric mercury transport and patterns of its deposition in both wet and dry processes. In this paper, current atmospheric mercury modeling techniques and the information obtained from them are described. A strategy for future field research and numerical model development is proposed which is intended to allow a confident identification of the sources of atmospheric mercury responsible for observed contamination of aquatic ecosystems.

Singh, R.B., and Huber, A.H. Development of a microscale emission factor model for CO for predicting real-time motor vehicle emissions. Journal of the Air & Waste Management Association 50 (11):1980-1991 (2000). EPA/600/J-00/323. 11/1/2000

Contact: William B. Petersen

Abstract:

Cooter, E.J., and Schwede, D.B. Sensitivity of the National Oceanic and Atmospheric Administration multilayer model to instrument error and parameterization uncertainty. Journal of Geophysical Research 105 (D5):6695-6707 (2000). EPA/600/J-01/060. 3/16/2000

Contact: William B. Petersen

Abstract: The response of the National Oceanic and Atmospheric Administration multilayer inferential dry deposition velocity model (NOAA-MLM) to error in meteorological inputs and model parameterization is reported. Monte Carlo simulations were performed to assess the uncertainty in NOAA-MLM deposition velocity estimates for ozone, sulfur dioxide, and nitric acid associated with measurements of meteorological variables (including temperature, humidity, radiation, wind speed, wind direction, and leaf area index). Summer daylight scenarios for grass, corn, soybean, oak, and pine were considered. Model sensitivity to uncertainty in the leaf area index (LAI), minimum stomatal resistance, and soil moisture parameterizations was explored. For sulfur dioxide and nitric acid, instrument error associated with the measurement of wind speed and direction resulted in the greatest velocity error. Depending on vegetation type, the most important source of uncertainty due to instrument error for the velocity of ozone was LAI. Of the model parameterizations studied, accurate estimation of temporal aspects of the annual LAI profile and the characterization of soil moisture supply and demand are most important to model-estimated velocity uncertainty. Considered individually, these factors can result in sulfur dioxide and nitric acid velocity estimate uncertainty of ?25% and ozone estimate uncertainty greater than 60%. For single plant species settings, reductions in estimate uncertainty should be possible with minor algorithmic modification, inclusion of more species-appropriate LAI profiles, and careful application of remote sensing technology.

Finkelstein, P.L., Ellestad, T.G., Clarke, J.F., Meyers, T.P., Schwede, D.B., Hebert, E.O., and Neal, J.F. Ozone and sulfur dioxide dry deposition to forests: observations and model evaluation. Published in: Journal of Geophysical Research 105 (D12):15,365-15,377 (2000). 6/27/2000

Contact: Peter L. Finkelstein

Abstract:

PUB REPORT

Atmospheric Modeling Division, and EPA Systems Development Center. Models-3 installation procedures for a PC with an NT operating system (Models-3 version 4.0). 2000. EPA/600/R-00/061 (NTIS PB2000-108511). 8/28/2000

Contact: Joan H. Novak

Abstract: Models-3 is a flexible software system designed to simplify the development and use of air quality models and other environmental decision support tools. It is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics. The June 2000 release of Models-3 contains a Community Multi-Scale Air Quality (CMAQ) modeling system for urban to regional scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The principal feature of this release is the ability to install and run Models-3 on a stand alone Windows-NT based computer. This Installation Manual includes an overview of the installation process, system requirements, procedures for installation of Models-3, and a description of system administration functions.

SYMPOS/CONF

Eder, B.K., Mebust, M.R., Binkowski, F.S., and Roselle, S.J. A preliminary evaluation of Models-3 CMAQ using visibility parameters. Presented at: International Symposium on the Measurement of Toxic and Related Air Pollutants, Research Triangle Park, NC, September 12-14, 2000. EPA/600/A-00/097 (NTIS PB2001-101445). 9/12/2000

Contact: Brian K. Eder

Abstract: Ambient air concentrations of fine particulate matter (PM 2.5) continue to be a major concern for the U.S. Environmental Protection Agency. High concentrations of fine particles have been linked to detrimental health effects (including an increase in mortality) and visibility degradation. Accordingly, the Clean Air Act and Amendment of 1990 called for an assessment of current and future regulations designed to protect human health and welfare. The most reliable tools for carrying out such assessments are air quality models like EPA's Community Multiscale Air Quality (CMAQ), which simulates air concentrations and deposition of PM 2.5 (along with other pollutants) and various measures of visibility associated with specified levels of emissions. These simulations can be used by EPA Program Offices and research laboratories to support both regulatory assessment and scientific studies on a myriad of spatial and temporal scales. This paper provides a preliminary evaluation of CMAQ using a visibility parameter called the deciview. The evaluation compares deciview values computed from visibility observations at 174 stations in the eastern half of the U.S. with those simulation by the model for the 5-day period July 11 - 15, 1995. Visibility was selected for this evaluation for two reasons: it can serve as a surrogate for PM 2.5, for which little observational data currently exist; and it has one of the most spatially and temporally comprehensive observational data sets available. The evaluation revealed a reasonable level of representation as CMAQ captured the basic spatial and temporal patterns of visibility degradation including major gradients and maxima/minima. The correlation coefficient between the observed and simulated deciviews for the entire simulation period was 0.56 and ranged from 0.38 on the 11th to 0.70 on the 13th. The model generally under predicted the visibility degradation by 10 deciviews; however, much of this discrepancy can be attributed to artifacts associated with the observed data.

Eder, B.K., Cohn, R.D., LeDuc, S.K., and Dennis, R.L. An aggregation and episode selection scheme for EPA's Models-3 CMAQ. Presented at: 12th Conference on Applied Climatology, Asheville, NC, May 8-11, 2000. EPA/600/A-00/077 (NTIS PB2001-100157). 5/8/2000

Contact: Brian K. Eder

Abstract: The development of an episode selection and aggregation approach, designed to support distributional estimation for use with the Models-3 Community Multiscale Air Quality (CMAQ) model, is described. The approach utilized cluster analysis of the 700 hPa u and v wind field components over the time period 1984-92 to define homogeneous meteorological clusters. Alternative schemes were compared using relative efficiencies and meteorological considerations. An optimal scheme was defined to include 20 clusters (five per season), and a stratified sample of 40 events was selected from the 20 clusters using a systematic sampling technique. The light-extinction coefficient, which provides a measure of visibility, was selected as the primary evaluative parameter for two reasons. First, this parameter can serve as a surrogate for PM-2.5, for which little observational data exist. Second, of the air quality parameters simulated by CMAQ, this visibility parameter has one of the most spatially and temporally comprehensive observational data sets. Results suggest that the approach reasonably characterizes synoptic-scale flow patterns and leads to strata that explain the variation in extinction coefficient and other parameters (temperature and relative humidity) used in this analysis, and therefore can be used to achieve improved estimates of these parameters relative to estimates obtained using other methods. Moreover, defining seasonally based clusters further improves the ability of the clusters to explain the variation in these parameters.

Pleim, J.A. A new land-surface model in MM5. Presented at: Tenth MM5 Users' Workshop, Boulder, CO, June 20-24, 2000. EPA/600/A-00/076 (NTIS PB2001-100182). 6/20/2000

Contact: Jonathan A. Pleim

Abstract: There has recently been a general realization that more sophisticated modeling of land-surface processes can be important for mesoscale meteorology models. Land-surface models (LSMs) have long been important components in global-scale climate models because of their more complete representation of the surface energy and moisture budgets as well as their ability to represent and respond to changing climatic conditions and changing ecosystems. For mesoscale meteorology modeling such long-term changes are not important, however, seasonal changes in vegetation and synoptic changes in surface moisture conditions have important effects on meteorological simulations. Surface processes, such as soil moisture and canopy conductance, control the partitioning of net radiation into sensible, latent, and ground heat fluxes which in turn have strongly influenced ground level air temperature and humidity as well as PBL development. Since these parameters are especially important for air quality modeling, inclusion of a sophisticated LSM is critical for air quality modeling studies. Furthermore, the dry deposition component of the air quality model can greatly benefit by direct use of LSM parameters such as bulk stomatal conductance and aerodynamic resistance.

Otte, T.L. Using MM5v3 with Eta analyses for air-quality modeling at the EPA. Presented at: Tenth MM5 Users' Workshop, Boulder, CO, June 20-24, 2000. EPA/600/A-00/087 (NTIS PB2001-100469). 6/20/2000

Contact: Tanya L. Otte

Abstract: Efforts have been underway since MM5v3 was released in July 1999 to set up air-quality simulations using Eta analyses as background fields. Our previous simulations used a one-way quadruple-nested set of domains with horizontal grid spacing of 108, 36, 12 and 4 km. With Eta analyses, it is anticipated that the 108-km domain (and possibly the 36-km domain) can be eliminated due to the better horizontal and vertical resolution of Eta compared to the 2.5 NCEP and ECMWF global analyses. In addition, it is anticipated that RAWINS can be eliminated from the processing pipeline since the 3-D variational analysis (3DVAR) technique used in the Eta Data Assimilation System (EDAS; Rogers et al. 1995) is widely considered to be superior to the Barnes technique used in RAWINS (Benjamin and Seaman 1985). That is, there may be little benefit to running RAWINS when the EDAS (theoretically) includes all of the observations that RAWINS could incorporate, and EDAS also ingests satellite, information. Since the operational and archived Eta domains and our 36-km simulation domain have comparable resolutions, it is hypothesized that the EDAS analyses would be appropriate to initialize our horizontal scale of interest.

Ching, J.K.S. Air quality modeling of PM and air toxics at neighborhood scales. Presented at: 11th Joint Conference on the Applications of Air Pollution Meteorology with the AWMA, Long Beach, CA, January 9-14, 2000. EPA/600/A-00/018 (NTIS PB2000-105756). 1/9/2000

Contact: Jason K. Ching

Abstract: The current interest in fine particles and toxics pollutants provide an impetus for extending air quality modeling capability towards improving exposure modeling and assessments. Human exposure models require information on concentration derived from interpolation of observations taken from monitoring networks. Causal mechanisms for adverse health from partiuclate matter and other air pollutants are numerous, but not well understood; however it provides much of the rationale for the nation's Pmresearch portfolio (NRC 98, 99). The NRC listed 10 causal hypotheses, each relating to some physical aspect or speciation of PM, and/or toxic pollutant species. The distribution of concentration fields for different PM causal pollutants will be highly complex at neighborhood scales. However, the number of locations of samplers of typical networks in urban areas is generally sparse; also, due to the sheer myriad of PM and toxic substances, temporal sampling of physical parameters of PM, speciated PM and toxic pollutants are limited and varied varying from sub-hourly to daily or weekly samples, and/or are surmised as surrogates of the available measurements. Thus, clearly, the observed temporal and spatial concentration fields are poorly, or inadequately resolved for driving exposure models and conducting health risk assessments. Currently the EPA emissions based modeling systems. Models-3 Community Multiscale Air Quality Modeling System (CMAQ) (Byun and Ching, 1999) is capable of modeling PM 2.5 and PM-10 at horizontal resolutions of ~36km for regional to 4 km for urban scale predictions. Urban areas are sources of large amounts of pollutants that contribute to significant and inherently subgrid spatial variability of the concentration fields and to subsequent exposures. Stationary monitors will be unable to characterize this variability. Current Eulerian-based air quality models' spatial resolution is coarse and cannot resolve the fine scale details. The modeling o

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Sugata, S., Byun, D.W., and Uno, I. Simulation of sulfate aerosol in east Asia using Models-3/CMAQ with RAMS meteorological data. Presented at: Millennium NATO/CCMS International Technical Meeting, Boulder, CO, May 16-19, 2000. EPA/600/A-00/032 (NTIS — 5/16/2000

Contact: Daewon W. Byun

Abstract: The present study attempts to address a few challenges in utilizing the flexibility of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. We apply the CMAQ system with the meteorological data provided by the Regional Atmospheric Modeling System (RAMS) and to a different geographical area, East Asia covering eastern half of China, Korean peninsula, and Japan Islands. To demonstrate the model performance, we compare the results with two time series of non-sea salt sulfate that are available at several sites in the southern part of Japan during January 1997.

Godowitch, J.M., and Young, J.O. Photochemical simulations of point source emissions with the Models-3 CMAQ plume-in-grid approach. Presented at: 93 Annual Meeting of AWMA Conference, Salt Lake City, UT, June 18-22, 2000. EPA/600/A-00/016 (NTIS PB2000-105757). — 6/18/2000

Contact: James M. Godowitch

Abstract: A plume-in-grid (PinG) approach has been designed to provide a realistic treatment for the simulation the dynamic and chemical processes impacting pollutant species in major point source plumes during a subgrid scale phase within an Eulerian grid modeling framework. The PinG science algorithms include a Plume Dynamics Model (PDM) processor and a Lagrangian plume module. The PDM processor generates plume dimensions and related parameters needed by the Lagrangian PinG module., which is an integral component of the Community Multiscale Air Quality (CMAQ) chemical transport model. PinG uses grid concentrations as boundary conditions and it provides an important feedback of plume pollutants to the grid in the appropriate grid cell when plume width reaches the grid cell size. Simulations were performed with the PinG treatment applied to point sources exhibiting a wide range of Nox emission rates situated in a regional modeling domain encompassing Nashville, Tennessee. Selected plume model results are presented from a case study day from Nashville/Middle Tennessee field study in June 1995. Modeled plume ozone and nitrogen species concentration evolved in the same manner found from observed plume data, which provides encouraging initial evidence of the capability of the PinG technique. The ozone recovery period in the modeled plume core and Nox oxidation were strongly dependent on the Nox emission rate. The excess ozone above background in the modeled plume was greater for point sources with higher Nox emissions.

Byun, D.W., and Pleim, J.A. Sensitivity of ozone and aerosol predictions to the transport algorithms in the Models-3 community multi-scale air quality (CMAQ) modeling system. Presented at: Millennium NATO/CCMS International Technical Meeting, Boulder, CO, May 16-19, 2000. EPA/600/A-00/010 (NTIS PB2000-107424). — 5/16/2000

Contact: Daewon W. Byun

Abstract: EPA's Models-3 CMAQ system is intended to provide a community modeling paradigm that allows continuous improvement of the one-atmosphere modeling capability in a unified fashion. CMAQ's modular design promotes incorporation of several sets of science process modules representing different algorithms and parameterizations of physical and chemical processes. For example, there are several different atmospheric transport algorithms available with CCTM. One objective of the present study is to demonstrate benefit of the modularity of the CMAQ system. Another is to assess the effects of different transport algorithms on air quality predictions. Here, we have demonstrated that the choice of modules in transport processes interacts with other model configurations.

Pleim, J.A., and Byun, D.W. Application of a new land-surface, dry deposition, and PBL model in the Models-3 community multi-scale air quality (CMAQ) model system. Presented at: Millennium NATO/CCMS International Technical Meeting, Boulder, CO, May 16-19, 2000. EPA/600/A-00/009 (NTIS PB2000-105969). 5/16/2000

Contact: Jonathan A. Pleim

Abstract: Like most air quality modeling systems, CMAQ divides the treatment of meteorological and chemical/transport processes into separate models run sequentially. A potential drawback to this approach is that it creates the illusion that these processes are minimally interdependent and that any meteorology model with a good reputation is adequate for air quality work. However, most mesoscale meteorology models are developed for operational weather forecasting and meteorological research. These foci do not emphasize all the same critical capabilities as air quality applications. Conversely, CTMs are often developed to accept basic meteorological inputs from a variety of sources with little regard to its quality and even less regard to consistency between physical parameterizations in the meteorology model and the CTM. The work reported here attempts to address some of these weak links in the system, particularly where improvements in land-surface modeling in the meteorology model and consistency with similar components in the CTM can have significant effects on the air quality simulation. Therefore, this development cuts across several system components. A new land-surface model (LSM), which features explicit simulation of soil moisture and vegetative evapotranspiration, has been coupled with the Fifth Generation Penn State/NCAR Mesoscale Model (MM5). An attendant dry deposition model has been developed to take advantage of the more sophisticated treatment of surface fluxes, stomatal conductance, and surface layer diffusion in the new LSM. The Meteorology Chemistry Interface Processor (MCIP) has been modified to include the new dry deposition model as well as to make the additional information resulting from the new LSM available to the CTM. Also, a new non-local closure PBL scheme that is compatible with the modifications made to the MM5 has been added to the list of vertical diffusion module options of the CMAQ CTM.

Kondragunta, S., Udelhofen, P.M., Schere, K.L., Roselle, S.J., and Holben., B. Attenuation of solar UV radiation by aerosols during air pollution episodes. Presented at: AMS Conference, Long Beach, CA, January 9-14, 2000. 1/9/2000

Contact: Kenneth L. Schere

Abstract: Increase in the amount of solar UV radiation reaching the surface due to decrease in stratospheric ozone continues to be a major concern (WMO, 1998). However, recent studies show that absorption and smattering by aerosols during air pollution episode decreases the amount of radiation reaching the surface (Dickerson el al.. 1997; Jacobson, 1998; Papayannis et al.. 1998; Repapis et al ..1998; Kondragunta et al.. 1999). To examine the role played by column ozone and aerosols in perturbing the solar radiation reaching the surface, we analyzed four years of spectrally resolved UV radiation measured by Brewer spectrophotometer at Gaithersburg, MD (39.1 N and 77.2 W). Transport from upwind regions and local pollution result in severe air pollution episodes at Gaithersburg when meteorological conditions are favorable. We present observations of aerosol optical depth and column ozone (from ground based sun photometers and satellites) and ground measurements of spectrally resolved UV flux. We will compare the observed and computed effects of aerosols on surface UV flux and discuss the implications.

Han, J., and Byun, D.W. A multi-stream model for vertical mixing of a passive tracer in the convective boundary layer. Presented at: 11th Joint Conference on the Applications of Air Pollution Meteorology with the AWMA, Long Beach, CA, January 9-14, 2000. EPA/600/A-99/091 (NTIS PB2000-102949). 1/9/2000

Contact: Daewon W. Byun

Abstract: We study a multi-stream model (MSM) for vertical mixing of a passive tracer in the convective boundary layer, in which the tracer is advected by many vertical streams with different probabilities and diffused by small scale turbulence. We test the MSM algorithm for investigating the effects of inhomogeneous mixing and vertical transport of multiple pollutants at different source heights in a three-dimensional air quality model. All input parameters in the MSM such as the probability density function and the mean updraft and downdraft are prescribed from large-eddy simulation (LES) data and the mixed-layer similarity theory. Applicability of the MSM is tested against the LES results for both near surface and elevated tracer sources. Results from the MSM compare well with those from LES for the overall temporal behavior of concentration distributions. However, a somewhat poor agreement between the MSM and the LES is seen in the magnitude of the concentrations at the surface and in the entrainment zone. It suggests that a further improvement of the MSM is needed to account for the frictional effects at the surface and the diffusion by small scale turbulence in the entrainment zone

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Presented Published

Cionco, R.M., Ellefsen, R.A., Huber, A.H., and Gallagher, J. An interdisciplinary approach to addressing neighborhood scale air quality concerns: the integration of GIS, urban morphology, predictive meteorology, and air quality monitoring tools. Presented at: 4th International Conference on Integrating GIS and Environmental Modeling (GIS/EM4): Problems, Prospects and Research Needs, Alberta, Canada, September 2-8, 2000. EPA/600/A-00/081 (NTIS PB2001-100188). 9/2/2000

Contact: William B. Petersen

Abstract: The paper describes a project that combines the capabilities of urban geography, raster-based GIS, predictive meteorological and air pollutant diffusion modeling, to support a neighborhood-scale air quality monitoring pilot study under the U.S. EPA EMPACT Program. The study has resulted in the establishment of a raster-based GIS urban morphology data set centered on Rodeo, CA and a large series of predictive microscale airflow (and diffusion) simulations in support of an operational mobile air quality monitoring system.

Streicher, J.J., Fornaro, R., Dulberg, M., Culverhouse, B., McConnell, A., Groce, M., King, K., and Price, A. "Modeling acute exposure to solar radiation." Paper presented at: 13th International Congress on Photobiology, Proceeding, 28th Annual American Society of Photobiology Meeting, Augusta, GA, July 1-6, 2000 7/1/2000

Contact: John J. Streicher

Abstract:

Huber, A.H., Bolstad, M., Freeman, M., Rida, S., Bish, I.E.S., and Kuehlert, K.H. Addressing human exposure to air pollutants around buildings in urban areas with computational fluid dynamics (CFD) Models. Presented at: AMS Third Symposium on the Urban Environment, Davis, CA, August 14-18, 2000. EPA/600/A-00/078 (NTIS PB2001-100156). 8/14/2000

Contact: William B. Petersen

Abstract: Computational Fluid Dynamics (CFD) simulations provide a number of unique opportunities for expanding and improving capabilities for modeling exposures to environmental pollutants. The US Environmental Protection Agency's National Exposure Research Laboratory (NERL) has been conducting cooperative research with Fluent, Inc. to examine and evaluate the application of CFD models for simulating air pollution along the pathway from source to human exposures. The basic framework of population-based human exposure models separates a person's day into time spent in a series of exposure microenvironments. The environmental concentration in these exposure microenvironments is weighted by the time-spent in each microenvironment to provide to a total daily exposure. The detailed spatial resolution of environmental pollution concentrations that is possible from CFD simulations can provide important information that is not available from a single point measurement. There are multiple potential roles for CFD simulations in supporting human exposure studies which will be presented outside of this brief abstract. In this study, we are examining in detail the urban buildings and roadway microenvironments of human exposure to ambient air pollutants. This abstract can present only a summary of some of the issues we are examining and a few examples of progress.

Schwede, D.B., LeDuc, S.K., and Otte, T.L. Using meteorological model output as a surrogate for on-site observations to predict deposition velocity. Presented at: Sixth International Conference on Air Surface Exchange of Gases and Particles, Edinburgh, England, July 3-7, 2000. EPA/600/A-00/079 (NTIS PB2001-100183). 7/3/2000

Contact: William B. Petersen

Abstract: The National Oceanic and Atmospheric Administration's Multi-Layer Model (NOAA-MLM) is used by several operational dry deposition networks for estimating the deposition velocity of O , SO , HNO , and particles. The NOAA-MLM requires hourly values of meteorological variables and since collection of on-site meteorology can be expensive, a study was performed to evaluate NOAA-MLM predicted deposition velocities using modeled meteorological data in lieu of on-site data. NOAA-MLM was run for three sites in the Clean Air Status and Trends Network using on-site data as well as the output of two mesoscale meteorological models, Eta and MM5. Atmospheric turbulence and local precipitation proved particularly difficult to match between the on-site and modeled data. Some modifications to the NOAA-MLM and the manner in which the Eta and MM5 data are processed my improve the usefulness of these data as a surrogate for the on-site observations.

Cooter, E.J., and Cohen, Y. Modeling flux pathways to vegetation for volatile and semi-volatile organic compounds in a multimedia environment. Presented at: Sixth International Conference on Air Surface Exchange of Gases and Particles, Edinburgh, England, July 3-7, 2000. EPA/600/A-00/080 (NTIS PB2001-100189). 7/3/2000

Contact: William B. Petersen

Abstract: This study evaluates the treatment of gas-phase atmospheric deposition in a screening level model of the multimedia environmental distribution of toxics (MEND-TOX). Recent algorithmic additions to MEND-TOX for the estimation of gas-phase deposition velocity over vegetated surfaces are evaluated via recently published dry deposition flux measurements. Model results are compared to similar estimates made by the NOAA multilayer dry deposition model. Results of the evaluation indicate that MEND-TOX performs quite well (r? = .74), for a screening level model, for the estimation of gas-phase dry deposition velocity of nitric acid over soybeans. As long as the stated model assumptions regarding chemical properties are met, the present study exceeds previous laboratory results for organic species to include some inorganic species and open field and dry leaf conditions.

Schwede, D.B., Petersen, W.B., and LeDuc, S.K. Simulating atmospheric exposure using an innovative meteorological sampling scheme. Presented at: Millennium NATO/CCMS International Technical Meeting, Boulder, CO, May 15-19, 2000. EPA/600/A-00/015 (NTIS PB2000-105755). 5/15/2000

Contact: William B. Petersen

Abstract: Multimedia Risk assessments require the temporal integration of atmospheric concentration and deposition estimates with other media modules. However, providing an extended time series of estimates is computationally expensive. An alternative approach is to substitute long-term average atmospheric estimates, but traditional methods for calculating long-term averages (e.g. joint frequency function) are not amenable to estimating wet deposition. In an effort to produce the required estimates without the computational burden, we developed an extension to the Sampled Chronological Input Model (SCIM) (Koch and Thayer, 1974) for use in U.S. Environmental Protection Agency's (USEPA) Industrial Source Complex - Short Term (ISCST3) model (USEPA, 1995). SCIM samples the long term meteorological record at regular, user-specified intervals. Since hourly meteorology is being used, the serial correlation between deposition and concentration and concentration is maintained. However, this simple sampling scheme significantly underestimates wet deposition, particularly at sites with frequent precipitation. We were able to reduce the uncertainty by introducing an additional sampling interval for hours with precipitation into the original SCIM methodology. Using this revised technique, concentration and dry deposition are calculated using the "regular" SCIM sampling; concentration and dry and wet deposition are calculated from hours sampled during "wet" SCIM sampling. A composite, weighted average is taken at the end of the simulation to determine annual values.

Huber, A.H., Rida, S., Bish, I.E.S., and Kuehlert, K.H. Addressing environmental engineering challenges with computational fluid dynamics. Presented at: 93rd Annual Meeting of AWMA Conference, Salt Lake City, UT, June 18-22, 2000. EPA/600/A-00/014 (NTIS PB2002-100867). 6/18/2000

Contact: William B. Petersen

Abstract: This paper discusses the status and application of Computational Fluid Dynamics)CFD) models to address environmental engineering challenges for more detailed understanding of air pollutant source emissions, atmospheric dispersion and resulting human exposure. CFD simulations provide a number of unique opportunities for expanding and improving capabilities for modeling environmental flows. The application of CFD for detailed modeling of environmental flows requires tools for complex geometry creation and meshing, advanced physical models and parallel computing capabilities. Unlike most currently used models, CFD simulations are able to account rigorously for topographical details such as terrain variations and structures in urban areas as well as local aerodynamics and turbulence. These features can be influential in determining local human exposures to environmental pollution. CFD simulations of complex distributions of pollutant concentrations within microenvironments of human exposure are feasible using today's high performance computing. Through further research, validation and testing, CFD modeling has the potential to become a reliable tool for estimating pollutant concentrations for situations that today have no reliable modeling method.

Discussions with examples are presented to highlight the use of CFD simulations as a tool or addressing environmental engineering problems. The ?basic steps' in developing a CFD application are presented. Particle attention is given to geometry modeling and meshing, the application of physical models and parameters (e.g., boundary conditions and turbulence models) and simulation post processing and evaluation.

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Singh, R.B., Huber, A.H., and Braddock, J.N. Modeling and measurement of real-time CO concentrations in roadway microenvironments. Presented at: 93rd Annual Meeting of AWMA Conference, Salt Lake City, UT, June 18-20, 2000. EPA/600/A-00/013 (NTIS PB2000-105754). 6/18/2000

Contact: William B. Petersen

Abstract: Although emission standards for motor vehicles continue to be tightened, tailpipe emissions continue to be a major source of human exposure to air toxics. The United States Environmental protection Agency's national Exposure Research laboratory has initiated a project to improve the methodology for modeling motor vehicle emissions from source through the pathway to human exposure. A real-time microscale automobile emission factor model for CO (MicroFacCO) virtually capturing all the information in the real world has been developed for United States vehicles. The model was developed for CO because of the available information to support its development. The goal is to use this CO model as a surrogate for other tailpipe air toxic emissions. The mission model is being used in conjunction with roadway dispersion models (e.g.,CALINE4), and being evaluated in the roadways around Research Triangle Park, North Carolina in a range of traffic fleet and meteorological conditions. Modeled concentrations are being compared with measured concentrations inside a moving vehicle and parked vehicle along the roadside. This paper discusses the new emission model, demonstrates the use of the emission model in modeling roadway air concentrations through an example, and discusses the issue and research needs for improving the methodology of modeling human exposures to mobile source emissions.

Brown, M.J., Lawson, Jr., R.E., DeCroix, D.S., and Lee, R.L. Mean flow and turbulence measurements around a 2-D array of buildings in a wind tunnel. Presented at: 11th Joint Conference on the Applications of Air Pollution Meteorology with the AWMA, Long Beach, CA, January 9-14, 2000. EPA/600/A-00/011 (NTIS PB2000-107423). 1/9/2000

Contact: Steven G. Perry

Abstract: In order to predict the dispersion of harmful materials released in or near an urban environment, it is important to first understand the complex flow patterns which result from the interaction of the wind with buildings and, more commonly, clusters of buildings. Recent advances in the application of computational fluid dynamics (CFD) models to such problems have shown great promise, but there is a need for high-quality data with which to evaluate (CFD) models. This study was performed to fill that need for a limited range of conditions.

High- resolution measurements of the three components of the mean and turbulent velocity statistics were obtained around a 2-D array of model buildings in the USEPA meteorological wind tunnel. In this paper, we briefly review prior field and laboratory experiments on building flows, describe our experimental set-up and measurement apparatus, present the flow measurements, and discuss their significance in relation to current understanding.

Wu, Y., Brashers, B., Pleim, J.A., and Finkelstein, P.L. "Development of a multilayer biochemical dry deposition model." Paper presented at: 24th Conference on Agriculture and Forest Meteorology American Meteorological Society, Davis, CA, August 13-14, 2000 8/13/2000

Contact: Peter L. Finkelstein

Abstract:

Finkelstein, P.L. Deposition velocities of SO2 and O3 over agricultural and forest ecosystems. Presented at: Sixth International Conference on Air Surface Exchange of Gases and Particles, Edinburgh, England, July 3-7, 2000. EPA/600/A-01/008 (NTIS PB2001-103692). 7/3/2000

Contact: Peter L. Finkelstein

Abstract: Abstract. The results of field studies that measured the flux and deposition velocity of SO2 and O3 are reported. Three of the studies were over agricultural crops (pasture, corn, and soybean), and two were over forest (a deciduous forest and a mixed coniferous - deciduous forest). In all cases the deposition velocity for SO2 was higher than that for O3. Diurnal cycles of SO2 deposition velocity were similar in shape, but not magnitude for all surfaces; however those for O3 showed some difference between forest sites where the peak was in the morning, and the agricultural sites where the peak occurred at mid-day. Seasonal cycles of SO2 were affected by deposition to surfaces when leaves weren't active, yet surface conductance is significant, but not for O3 where stomatal uptake is the primary pathway for deposition.

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Presented Published

Arnold, J.R., and Dennis, R.L. First results from operational testing of the U.S. EPA Models-3 community multiscale model for air quality (CMAQ). Presented at: Millennium NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 15-19, 2000. EPA/600/A-01/020 (NTIS PB2001-104132). 5/15/2000

Contact: Robin L. Dennis

Abstract: The Models 3 / Community Multiscale Model for Air Quality (CMAQ) has been designed for one-atmosphere assessments for multiple pollutants including ozone (O3), particulate matter (PM10, PM2.5), and acid / nutrient deposition. In this paper we report initial results of our evaluation of the model's operational performance for O3 for the northeast U.S. over the 14 day period 5?18 July 1995 with three one-way nested model resolutions at 36km, 12km, and 4km and using two chemical mechanisms, CB4 and RADM2. We defined subdomains with similar photochemical regimes within the modeled domains by analysis of 1995 surface observations, and within these subdomains we segregated airsheds for the large urban areas. CMAQ model performance was evaluated over a number of specific attributes including the ability to reproduce the 1 hour peak and the 3 hour and 8 hour average daily maximum O3 mixing ratios [O3], and the ability to reproduce diurnal profiles of O3 and oxides of nitrogen (NO+NO2=NOX). Statistical results for the 8 hour average maximum [O3] are quite similar to those for the 1 hour peak and 3 hour average. Normalized bias and gross error statistics show that CMAQ does quite well on high [O3] days, but less-well on lower [O3] days and on days with larger mean-to-maximum ranges. One possible explanation is that this O3 performance difference is tied to the model's inability to predict NOX correctly for low O3 days. We find that the 36km grid is likely too coarse for most city and some regional model applications. The 12km model is an improvement nearly everywhere nearly every day as measured by the bias and error statistics. Statistics for the 4km model demonstrate a tendency for improved fits over the12km but this is not so ubiquitous as for the 12km over the 36km. The improvements across grid resolutions measured with bias and error statistics are not uniformly seen when plotting diurnal time series of the different model resolutions against observations at a given site. This most likely indicates significant problems of monitor siting and representativeness for a model cell. Both bias and error and most diurnal profiles in the [O3] results for the CB4 chemistry are quite similar to those obtained with the RADM2 chemistry for most days in most regions and cities. Comparisons to HCHO observations constitute a special test for the model since the chemical mechanisms were not originally designed or fitted to predict HCHO. CMAQ predictions of [HCHO] at both 36km and 12km with CB4 and with RADM2 demonstrate a fairly good fit to the 3-hour averaged observed [HCHO] reported for several PAMS sites in the northeast. Our overall conclusion for this first operational evaluation of CMAQ is that the model is for the most part functioning in a way we can account for both where model fits to the observations are good and where they are not as good. Furthermore, we find that CMAQ is operating well-within the range of results from other large, ozone-only Eulerian AQMs in the U.S. for the high O3 days where model evaluation has traditionally been focused. Hence we find no reason not to use the model and encourage its wide-spread use.

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Abstract: The complexity of environmental problems we face now and in the future is ever increasing. Process linkages among air, land, surface and subsurface water require interdisciplinary modeling approaches. The dynamics of land use change spurred by population and economic growth, and the impact of Best Management Practices in urban and agricultural areas must be considered in environmental exposure and risk assessments. An abundance of related research and model development is proceeding in Universities, Federal agencies and research laboratories, and related research is being sponsored by industry-based research foundations. Thus, one of the primary goals of this workshop is to bring together stakeholders from many of these diverse groups for exchange of information about their modeling needs and research activities with special emphasis on techniques, tools, and frameworks for model integration, characterization of landscape and subsurface features, and data visualization and analysis tools. EPA is interested in fostering a "community approach" to multi-disciplinary ecosystem modeling and analysis. The emerging problems are larger than one group or one agency can expect to solve, so our goal is to work together toward open-architecture problem solving environments that facilitate the integration of state-of-the-science process models/modules, application domain specification and data preparation, and decision support. A flexible Problem Solving Environment will enable exploration of a variety of modeling approaches dealing with multiple scale and stressor interactions. Object technology, new computing algorithms and architectures, and intelligent data analysis techniques offer promise for overcoming previous computing limitations and modeling inflexibility. During the workshop, investigators from the 1996 EPA STAR grants for High Performance Computing and Communications will be presenting the results of their three year research efforts, and investigators for the 1999/2000 EPA STAR grants for Computing Technology for Ecosystem Modeling will be presenting their research directions for the next three years. Numerous other researchers and stakeholders engaged in ecosystem modeling and monitoring will also be presenting progress-to-date on their projects. The anticipated outcomes of the workshop are better understanding of 1) cross-media exchange processes and scale issues, 2) a variety of framework approaches for dealing with cross-discipline model integration and application issues, and 3) identification of inter-disciplinary opportunities for collaboration.